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MODEL OF DIRECT INITIATION OF
UNCONFINED DETONATIONS

S. EIDELMAN
NATIONAL RESEARCH COUNCIL
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NAVAL POSTGRADUATE SCHOOL

Monterey, California

Rear Admiral J. J. Ekelund
Superintendent

D. A. Schrady
Acting Provost

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W. M. TOLLES
Dean of Research

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An analytical model of the direct initiation of detonation waves with planar, cylindrical, and spherical symmetry is developed. This model shows that the energy requirements for the self-sustained detonation wave differ significantly for planar, cylindrical and spherical detonations. The new concept of minimum compensation energy was introduced and the technique of calculation of minimum initiation energy was developed. The results are verified by numerical simulation of the full governing equations and by comparison to experimental data.

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I. Introduction

Direct initiation of the self-sustained detonation was first studied experimentally using the shock tube technique, where both the initiating shock and the detonation wave had a planar symmetry[1]. Attempts to apply the results of these experiments to predict the detonation threshold in the cases of spherical or cylindrical detonations failed. This led to experimental studies of the influence of the ignition source geometry on the initiation process[2] and to full-scale experiments to study the threshold for the direct initiation of unconfined spherical[3,4] and planar[5] detonations in gaseous mixtures. These studies showed the strong influence of the geometry of the ignition source on the threshold for direct initiation. For example, although Bull et al.[3], failed to achieve detonation in methane-air using a strong spherical blast, Benedick[5], achieved detonation in the same mixture using planar initiation.

In this study we propose a simple model that permits exploration of the influence of the symmetry of the initiation process on the direct initiation threshold.

II The Model of the Energetic Deficit of the Initiation Process

The direct initiation of an unconfined, stable detonation wave can occur under certain specific conditions. One of the main conditions is generation of a supersonic compression front of sufficient strength to initiate fast exothermal reactions in the medium. The energy released in these exothermal reactions must be sufficient to compensate for the energy density lost through

hydrodynamic expansion and for the work done on the surrounding medium.

Let us assume that both these conditions have been met at a large distance from the initiation region and that the self-sustained detonation wave is propagating with a constant velocity through the combustible medium. It is obvious that if the detonation wave is distant enough from the initiation region, its parameters are not dependent on the symmetry of the wave or on the reaction zone length. Moreover, its parameters could be found with very good accuracy using Chapman-Jouguet's theory, which does not consider any one of these factors. On the other hand, if the initiation source produces in it vicinity a supersonic compression front of sufficient strength to initiate fast exothermal reactions, this is not a sufficient condition for direct initiation of the self-sustained detonation wave. The experimentally determined, minimum critical energy needed for direct initiation varies by three or more orders of magnitude for different fuels and for initiation sources of different geometry. The initiation energy is larger than that required to produce the supersonic compression front necessary for initiation of fast chemical reactions in the medium.

Why, in most cases, is the achievement of the necessary conditions for initiation not sufficient for the formation of the self-sustained detonation wave? This question leads to the concept that in most cases the energy of combustion required for self-sustained detonation waves is a function of the distance from the initiation source.

Figure 1 shows the pressure distribution behind the front of a typical detonation wave. The region behind the wave front is divided into two zones. Zone I lies from the radius $r = 0$ up to the Chapman-Jouguet point. Zone II is between the Chapman-Jouguet point and the front of the detonation wave. Let us estimate the energy which is contained in each of these zones.

We now consider the self-sustained detonation wave. Its parameters and the structure of the wave shown in Figure 1 do not change over time. If the kinetic energy of Zone 1 is neglected (because the mass velocity of the gas is very low in this region) and the average pressure is taken equal to 1.25 x P (see Figure 1), then the energy of Zone I:

$$E_I = \frac{1}{\nu}\sigma_\nu S\left(\frac{1.25\ P}{\gamma-1}\right) r_1^{\ \nu} \qquad (1)$$

where $\nu = 1, 2, 3$ for planar, cylindrical and spherical symmetries.

$\sigma_\nu = 2(\nu-1)\pi + (\nu-2)(\nu-3)$

$S = 1m^{(3-\nu)}$

The kinetic energy of Zone II should be considered. Let us assume it to be the average between the kinetic energy at the shock front and the kinetic energy at the Chapman-Jouguet plane. Let us also assume that the pressure in Zone II is equal to the average of the pressure immediately behind the shock front and at the Chapman-Jouguet plane. These assumptions yield an approximate value of 2.5 x P . Zone II energy then will be:

$$E_{II} = \frac{1}{\nu}\,\sigma_\nu S\left(\frac{2.5\,P}{(\gamma-1)} + \frac{\rho_{cJ}V_{cJ}^{\,2} + \rho_{sh}V_{sh}^{\,2}}{4}\right)(r_2^{\,\nu} - r_1^{\,\nu}) \tag{2}$$

where ρ_{cJ} , V_{cJ} - density and the mass velocity of the gas at the Chapman-Jouguet point.

ρ_{sh} , V_{sh} - density and the mass velocity of the gas immediately behind the shock front.

Let us now calculate the energy increment of Zone I, when the wave radius increases by Δr :

$$\Delta E_I = 2S\,\frac{P\,1.25}{(\gamma-1)}\,\Delta r \text{ , when } \nu = 1 \tag{3a}$$

$$\Delta E_I = \pi S\,\frac{P\,1.25}{(\gamma-1)}\,(2\Delta r r_1 + \Delta r^2) \text{ , when } \nu = 2 \tag{3b}$$

$$\Delta E_I = \frac{4}{3}\pi\,\frac{P\,1.25}{(\gamma-1)}\,(3r_1^{\,2}\Delta r + 3r_1\Delta r^2 + \Delta r^3) \text{ , when } \nu = 3 \tag{3c}$$

The energy increment of Zone II when the detonation wave radius increases by Δr will be:

$$\Delta E_{II} = 0 \quad \text{when } \nu = 1 \tag{4a}$$

$$\Delta E_{II} = \pi SA(2\Delta r r_2 - 2\Delta r r_1) \quad \text{when } \nu = 2 \tag{4b}$$

$$\Delta E_{II} = \frac{4}{3}\pi A[3\Delta r^2(r_2 - r_1) + 3\Delta r(r_2^{\,2} - r_1^{\,2})] \quad \text{when } \nu = 3 \tag{4c}$$

where $$A = \left(\frac{2.5\,P}{\gamma-1} + \frac{\rho_{cJ}V_{cJ}^{\,2} + \rho_{sh}V_{sh}^{\,2}}{4}\right)$$

Let us now calculate the limit of the ratio between the total energy behind the detonation wave and the energy of the Zone I when $\Delta r \to 0$:

$$F_1(r_1, L) = \lim_{\Delta r \to 0} \frac{E_I + E_{II}}{E_I} = 1 \text{ , when } \nu = 1 \tag{5a}$$

$$F_2(r_1, L) = \lim_{\Delta r \to 0} \frac{E_I + E_{II}}{E_I} = 1 + \frac{A(\gamma - 1)}{P\ 1.25} \frac{L}{r_1} \text{ ,} \quad \text{when } \nu = 2 \tag{5b}$$

$$F_3(r_1, L) = \lim_{\Delta r \to 0} \frac{E_I + E_{II}}{E_I} = 1 + \frac{A(\gamma - 1)}{P\ 1.25} \left(\frac{2L}{r_1} + \frac{L^2}{{r_1}^2}\right) \text{ ,} \quad \text{when } \nu = 3 \tag{5c}$$

where $L = r_2 - r_1$, the reaction zone length.

We conclude from Equations 5a, 5b and 5c that the energy requirements for the self-sustained detonation wave vary according to the symmetry of initiation. In the case of planar symmetry, the energy requirement is not dependent on the distance from the initiating source and the length of the reaction zone. For this reason the direct initiation of the planar detonation must be easier to attain. In the planar case it is sufficient to produce a supersonic compression front capable of initiating fast exothermal reactions to form a self-sustained detonation wave.

In the case of spherical symmetry, as Equation 5c shows, the energy required for self-sustained detonation varies with radius r_1 and with reaction zone length L . At a large

distance from the initiation source, the energy release of the medium is equal to the amount of energy needed to support the self-sustained detonation wave, according to Chapman-Jouguet's theory and $\lim_{r_1 \to \infty} F_3(r_1, L) \to 1$. In the region close to the initiating source, the $F_3(r_1, L)$ value can be considerably larger than 1. For example if $L = 1cm$; $r_1 = 10cm$ and $\frac{A(\gamma-1)}{P\ 1.25} = 2$ (which is a minimum estimate not taking into account the kinetic energy of the gas), then $F_3 = 1.42$. This means that to support the self-sustained detonation wave at the constant level, the energy released from the medium at the radius 10 cm must be 42% larger than what is required at a very large distance from the source.

If in the cases of cylindrical and spherical symmetry the density of the chemical energy released by the medium is constant, the propagating detonation wave will have an energetic deficit which decreases when the radius of the wave increases. This phenomena is responsible for the decay of the detonation wave in the initiation source region. If this decay does not bring to an end rapid combustion in the reaction zone, the detonation wave, after reaching its minimum value, is gradually accelerated towards the Chapman-Jouguet detonation velocity of the mixture. This was observed experimentally by Bar- Or, et al.[6] for cylindrical symmetry and by Atkinson, et al.[7] for spherical symmetry. It should be noted here that this kind of detonation wave behaviour was not observed in the shock tube experiments, where the detonation is planar.

Mitrofanov, et al.[8], Eidelman and Burcat[9], and Eidelman and Sichel[10], all have simulated detonation wave decay and acceleration in two-phase media. In these works[9,10], the value of the detonation wave parameters of the minimum point were found to be inversely dependent on the reaction zone length, which is in qualitative agreement with Equation 5c, where increase of the reaction zone length leads to increase of the energetic deficit or, in other words, decrease of the detonation wave.

III. Test of the Model of Energetic Deficit

When a detonation wave is initiated in a two-phase medium the energetic deficit should be greater than that of the gaseous phase detonation, because the reaction zone length is usually larger in the former than in the latter. Numerical modeling of spherical two-phase detonation, initiation, and propagation shows decay of the detonation wave to the minimum value point. In some cases the pressure immediately behind the shock front is half that of the Chapman-Jouguet detonation wave[9,10].

A series of numerical simulations was carried out to test qualitatively and quantitatively the model of energetic deficit, using the computer code for the two-phase detonation[9,10,11].

For the numerical simulation two kinds of combustible media were chosen:

a) stoichiometric mixture of oxygen and decane droplets with diameter 120μ.

b) stoichiometric mixture of oxygen and decane droplets with diameter 300μ.

The reaction zone length for these mixtures differs by approximately one order of magnitude during the initiation process. This difference allows us to evaluate the influence of this parameter on the model of energetic deficit.

For each of these mixtures, three kinds of numerical simulations were performed:

I Initiation and propagation of a planar detonation wave.

II Initiation and propagation of a spherical detonation wave.

III Initiation and propagation of a spherical detonation wave with compensation for energetic deficit. In this case the energy released behind the shock front was assumed to follow Equation 5c. That means that compensation for the energetic deficit in the initiation region was done by artificially increasing the thermal effect of the chemical reaction per unit mass of fuel according to Equation 5c.

The results of these simulations are presented in Figure 2, which shows plots of detonation wave velocity versus shock radius. In cases of spherical symmetry the energy of the igniting explosion was equal to 156000J, while in cases of planar symmetry the corresponding value was 3×10^6 J/m^2 . The velocity of the Chapman-Jouguet detonation was calculated for a stoichiometric gaseous mixture of decane and oxygen using the Gordon-McBride program[12]. The calculated Chapman-Jouguet value is noted on the velocity scale of Figure 2.

Figure 2 reveals quite clearly that, in cases of planar detonation the initiation process proceeds without a significant region of decay. Beyond 0.6m curves 1 and 2 coincide, regardless

of differences in the reaction zone length (2cm for Case 1 and 6cm for Case 2). The velocity of the detonation wave for Case 1 is equal to the Chapman-Jouguet detonation velocity of the mixture at a distance of 0.2m from the initiating source. In Case 2 the C-J velocity is reached at a distance of 0.6m. After initiation the wave decays up to 5% below the C-J velocity value. This can be explained by the energetic dificit caused by changes in the detonation wave structure, which are not considered in Equations (5a, 5b and 5c) and which are larger in Case 2 because of the greater reaction zone length.

In Cases 5 and 6 spherical detonation was initiated in mixtures "a" and "b". In accordance with the significant energetic deficit predicted by Equation 5c, the detonation wave decayed far below the C-J velocity. After reaching it's minimum value the detonation wave accelerated slowly.

The decay is much greater in Case 6, because the reaction zone length is larger. This is in accord with Equation 5c, which holds that reaction zone length and energetic dificit are directly proportional to one another.

In Cases 3 and 4 the energetic deficit of the spherical detonation initiation process was compensated for in accordance with Equation 5c. Figure 2 reveals that the energy released in accordance to Equation 5c completely compensated for the energetic deficit of the initiation process. The detonation wave in these cases does not decay below 5% of the C-J velocity and steady-state detonation with the velocities close to the C-J velocity value are achieved at a distance of 0.3 - 0.4m from the initiation source.

In the process of testing the energetic deficit model, the energy of Zones I and II was calculated. In the case of planar detonation, the energy of Zone II is constant beyond a radius of 0.25m for Case 1, and 0.5m for Case 2, which is consistent with Equation 5a.

In Cases 3 and 4, when the energetic deficit was artificially compensated for, the actual ratio of the energies of Zone II and I differed by only 5% to 13% from those predicted by Equation 5c.

Thus, Equation 5c gives a very good approximation of the energetic deficit of the initiation process in cases of spherical detonation.

IV Calculation of the Energy for Direct Initiation, Using the Energetic Deficit Model

For direct initiation of the self-sustained detonation wave, the energetic deficit of the initiation process of spherical and cylindrical detonations is usually compensated for by increasing the igniting source energy. The increase in the energy released by the igniting source increases the radius of the region of the overdriven detonation wave. This permits initiation of a self-sustained detonation wave beyond the radius where the energetic deficit given by Equations 5b and 5c is small and does not result in the complete decay of the detonation wave.

The determination of the threshold for the direct initiation of the self-sustained detonation is of significant applied interest. The Equations 5a, 5b and 5c provide a new technique for calculating the minimum initiation energy.

For calculation of the minimum initiation energy in the cases of spherical and cylindrical detonations, let us introduce a new concept - minimum compensation energy. Minimum compensation energy is the minimum additional energy needed to be released in the process of direct initiation of spherical or cylindrical detonations. This energy extends the radius of the overdriven detonation to the point where the energetic deficit given by Equations 5b and 5c does not lead to the complete decay of the detonation wave.

The minimum compensation energy can be calculated using Equations 5a, 5b and 5c.

For cylindrical symmetry it is given by:

$$E_{c2} = 2\pi \int_{r_o}^{r_c} \left[F_2 \,(r_1, L) - F_1 \right] Q \, r_1 dr_1 = 2\pi \int_{r_o}^{r_c} \frac{A(\gamma-1) L \, Q}{P \;\; 1.25} \, dr_1 \tag{6a}$$

For spherical symmetry it will be:

$$E_{c3} = 4\pi \int_{r_o}^{r_c} \left[F_3 \,(r_1, L) - F_1 \right] Q \, r^2 dr$$

$$= 4\pi \int_{r_o}^{r_c} \frac{A(\gamma-1)}{P \; 1.25} \left(\frac{2L}{r_1} + \frac{L^2}{r_1{}^2} \right) Q \, r_1{}^2 dr_1 \tag{6b}$$

where E_{c2}, E_{c3} - minimum compensation energy for cylindrical and spherical symmetry, respectively;

r_o - initiating source radius;

r_c - minimum compensation radius

Q - heat release per unit volume for the stoichiometric mixture

If it is assumed that the detonation wave parameters do not change during the initiation process the minimum compensation energy can be simply calculated:

$$E_{c2} = 2\pi \frac{A(\gamma-1)}{P\ 1.25} Q\ L(r_c - r_o) \tag{7a}$$

$$E_{c3} = 4\pi \frac{A(\gamma-1)}{P\ 1.25} Q \left[L\left(r_c^{\ 2} - r_o^{\ 2}\right) + L^2\left(r_c - r_o\right)\right] \tag{7b}$$

The minimum energy behind the initiation source radius r_o must be of sufficient magnitude to generate a supersonic compression front sufficiently strong to initiate fast exothermal reactions in the medium. The minimum initiation energy can be determined from:

$$E_{min} = E_{ci} + E_o \tag{8}$$

where $i = 2, 3$

E_o - energy release behind the radius r_o

The value of r_o must be larger than the reaction zone length - L. With this information the minimum value of E_o in Equation 8 can be found.

The value of E_{ci} can be determined if the minimum compensation radius r_c is known. According to our definition the energetic deficit at radius v_c from the initiation source is small and a self-sustained detonation wave can propagate in the mixture at radius r_c regardless the energetic deficit.

For example, let us calculate the minimum energy required for the direct initiation of a spherical detonation wave in a methane/air mixture. The reaction zone length of this mixture for the Chapman-Jouguet detonation according to Burcat, et al[13] is $L \simeq 0.20m$. Let us assume that the self-sustained detonation wave can propagate in this mixture when the energetic deficit is less than or equal to 5% of the heat of the stoichiometric methane - air combustion. The r_c value can be calculated from:

$$\frac{A(\gamma-1)}{P\ 1.25}\left(\frac{2L}{r_c} + \frac{L^2}{r_c^{\ 2}}\right) = 0.05 \qquad (9)$$

$\frac{A(\gamma-1)}{P\ 1.25} \simeq 2$, if we neglect the kinetic energy of gas in the zone II (see Figure 1). Then solving Equation 9 we obtain:

$$r_c \simeq 16.1m$$

If $r_o = 0.2m$, E_{c3} can be calculated from Equation 7b:

$$E_{c3} \simeq 4.7x10^9 \ J$$

In this case the value of E_o is negligible compared to the value of E_{c3} . For this reason $E_{min} \simeq 4.7x10^9$ J . This value is one order of magnitude larger than the value obtained by Matsui and Lee[2].

V Discussion and Conclusions

The theory developed here verifies that the process of direct initiation of the detonation wave differs significantly for planar, spherical, or cylindrical detonations. The energy

requirements for the self-sustained detonation wave in the planar case does not change in the medium surrounding the initiator. In spherical and cylindrical detonations the energy requirement for the self-sustained detonation wave is a function of both the distance from the initiator and the reaction zone length.

In this study the analytical expressions representing the energetic deficit of the initiation process were found. By a series of numerical experiments it was shown that compensation for the energetic deficit in accordance with the analytically determined function resulted in the spherical and planar initiation processes to evolve similarly.

In the course of exploring of the theory developed here the concept of minimum compensation energy was introduced. Although only the qualitative definition of this concept is given, it is useful for better understanding of the initiation process in spherical and cylindrical detonations. The formulated concept of minimum compensation energy allows one to calculate the minimum initiation energy for spherical and cylindrical detonations, when the minimum compensation radius r_c is known. More work is needed to define quantitatively r_c, which probably could be determined on the basis of shock-tube kinetic data.

Analysis of equations 7a, 7b and 8 shows that in cases where the self-sustained detonation wave is formed only in the region where the energetic deficit is very small, the initiation energy required will be very large. In other words, narrowing the detonability limits of spherical or cylindrical detonations causes an increase of initiation energy. An increase in the

reaction zone length also causes increase of initiation energy. It follows, then, that in mixtures with large reaction zone lengths and narrow detonability limits spherical and cylindrical detonation will be very difficult to initiate, because of large energetic deficit of the initation process.

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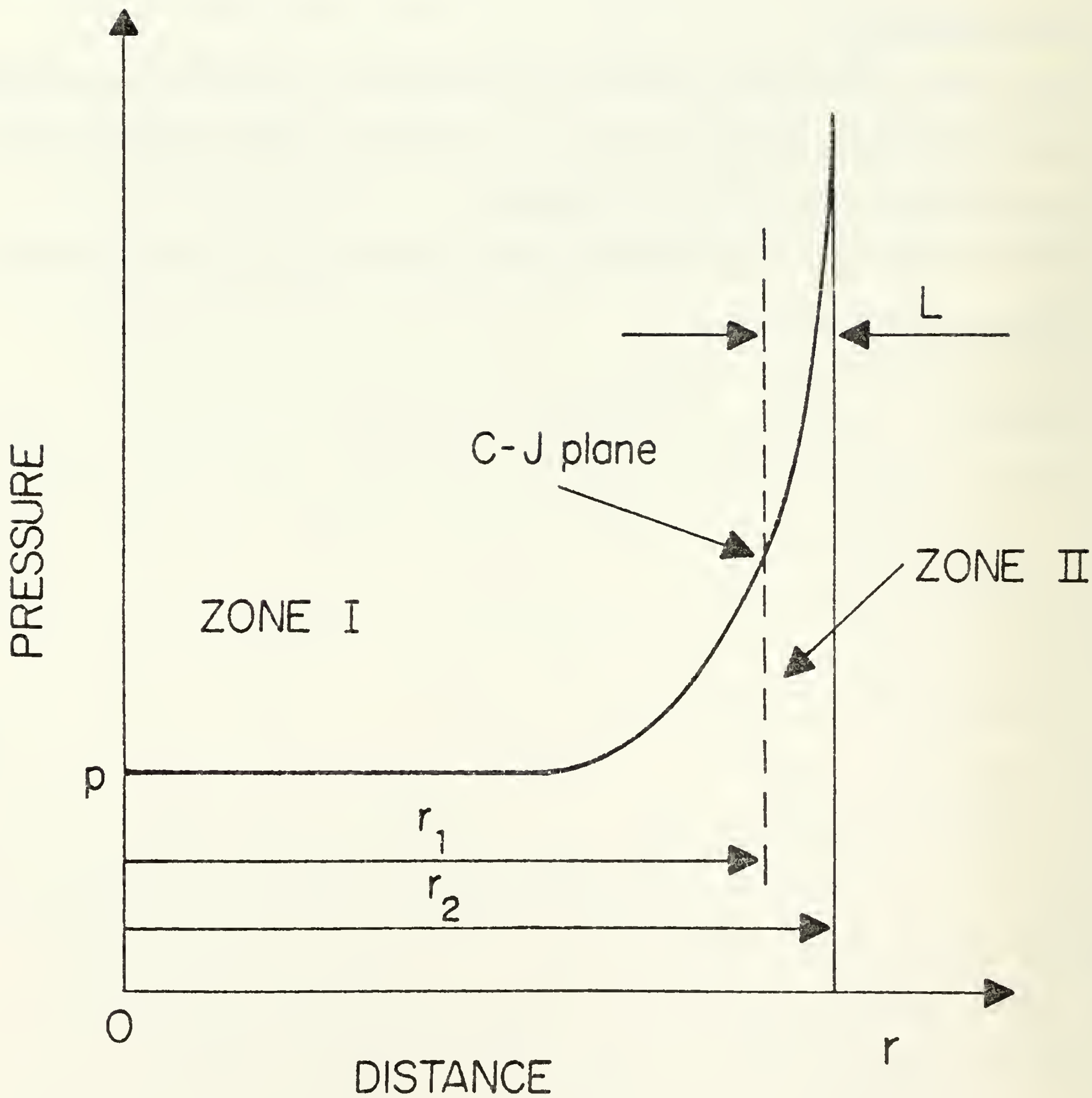

Figure 1. The structure of the self-sustained detonation wave. The pressure distribution.

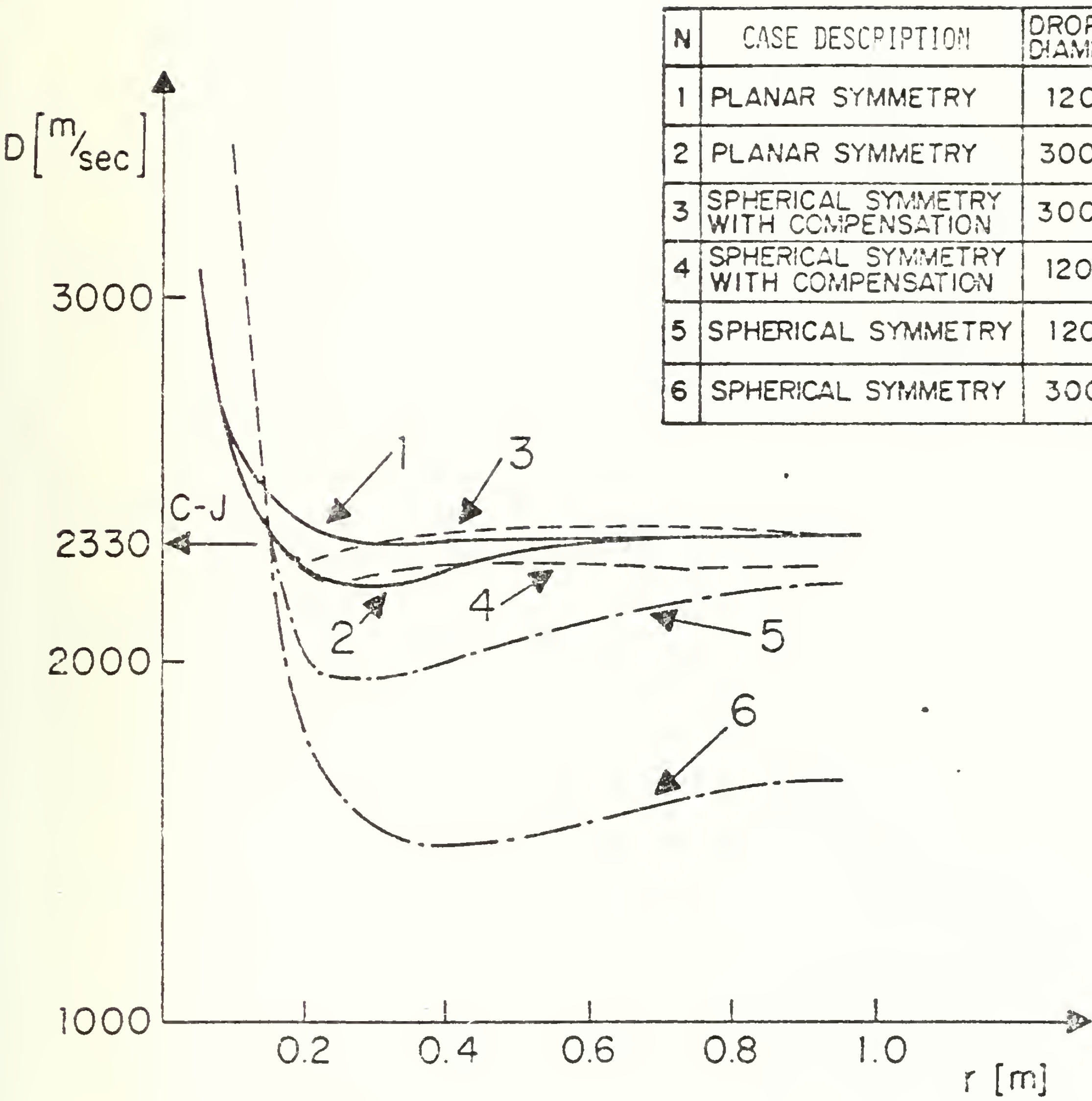

Figure 2. The detonation wave velocity versus shock radius.

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